Markov chain Monte Carlo idea

⋆ Situation:

– Given a target distribution $f(x)$

– Want to estimate

$$\mu = \mathrm{E}_f[g(X)] = \int g(x)f(x)\mathrm{d}x$$

– Want to generate samples from $f(x)$

⋆ Idea:

– construct a Markov chain $\{X_i\}_{i=1}^{\infty}$ so that

$$\lim_{i\to\infty} P(X_i = x) = f(x)$$

– simulate the Markov chain for many iterations

– for m large enough $x_m, x_{m+1}, \ldots$ are (essentially) from $f(x)$

– estimate μ by

$$\widetilde{\mu} = \frac{1}{n}\sum_{i=m}^{m+n-1} g(x_i)$$

Markov chain Monte Carlo: questions to answer

- ⋆ Questions to answer:
  - how to construct such a Markov chain?
  - how to simulate the Markov chain?
  - how to find the value of m?
  - how to estimate $\mathrm{Var}[\widehat{\mu}]$?

Markov chain Monte Carlo: questions to answer

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  - how to construct such a Markov chain?
  - how to simulate the Markov chain?
  - how to find the value of m?
  - how to estimate $\text{Var}[\widehat{\mu}]$?

- How to construct such a Markov chain? ($x \in \Omega$ discrete)
  - Markov chain transition probabilities: $P(y|x) = P(X_{i+1} = y | X_i = x)$
  - Need to have

$$f(y) = \sum_{x \in \Omega} f(x) P(y|x) \quad \text{for all } y \in \Omega$$

  - Sufficient condition: Detailed balance condition

$$f(x) P(y|x) = f(y) P(x|y) \quad \text{for all } x, y \in \Omega$$

Metropolis–Hastings

⋆ Detailed balance condition:

$$f(x)P(y|x) = f(y)P(x|y) \quad \text{for all } x, y \in \Omega$$

⋆ Metropolis–Hastings setup for $P(y|x)$:

$$P(y|x) = Q(y|x)\alpha(y|x) \ \text{ when } y \neq x$$

$$P(x|x) = 1 - \sum_{y \neq x} Q(y|x)\alpha(y|x)$$

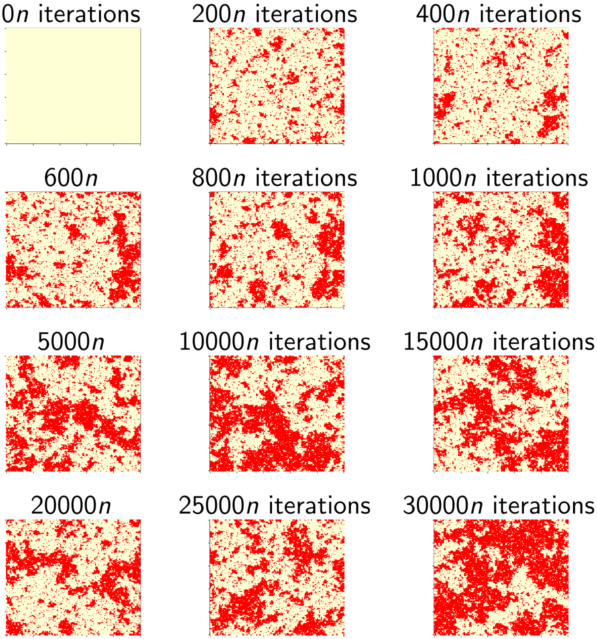
where

- $Q(y|x)$ is a transition matrix (proposal kernel)
- $\alpha(y|x) \in [0,1]$ is an acceptance probability

⋆ Questions:

- how to simulate the Markov chain with this setup?
- for given $Q(y|x)$, what can $\alpha(y|x)$ be?

Ising model ($\beta = 0.87, x^0 = 0$



Ising model

⋆ Trace plot of number of 1's

- four runs
- different initial state:
  + all 0's
  + all 1's (two runs)
  + independent random in each node